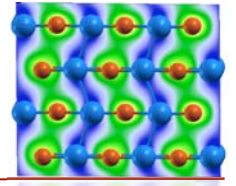


Computational Materials Science Seminar



Extended Born-Oppenheimer Molecular Dynamics

Speaker: Dr. Anders Niklasson

Theoretical Division, Los Alamos National Laboratory

Time: Clark 609, 2:30-3:30 pm, Thursday, May 1

Abstract:

A Lagrangian generalization of time-reversible Born-Oppenheimer molecular dynamics [Niklasson et al., Phys. Rev. Lett. vol. 97, 123001 (2006)] is presented. The Lagrangian includes extended electronic degrees of freedom as auxiliary dynamical variables in addition to the nuclear coordinates and momenta. While the nuclear degrees of freedom propagate on the Born-Oppenheimer potential energy surface, the extended auxiliary electronic degrees of freedom evolve as a harmonic oscillator centered around the adiabatic propagation of the self-consistent ground state. The formulation enables the application of higher-order symplectic or geometric integration schemes that are stable and energy conserving even under incomplete self-consistency convergence. I will demonstrate how the extended Born-Oppenheimer molecular dynamics improves the accuracy by over an order of magnitude compared to previous formulations at the same level of computational cost.

Host: Richard G. Hennig **Organizers:** T. Arias, G. Chan, R. Hennig, C. Umrigar

The Computational Materials seminars are held on the 1st and 3rd Thursdays of each month and provide an informal setting for internal and external speakers to present works on materials simulation and other theoretical aspects of materials.

Sponsorship:

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